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Uncertainty quantification for complex systems with very high dimensional response using Grassmann manifold variations

D.G. Giovanis, M.D. Shields *

Department of Civil Engineering, Johns Hopkins University, Baltimore, MD 21218, USA

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ABSTRACT

This paper addresses uncertainty quantification (UQ) for problems where scalar (or low-dimensional vector) response quantities are insufficient and, instead, full-field (very high-dimensional) responses are of interest. To do so, an adaptive stochastic simulation-based methodology is introduced that refines the probability space based on Grassmann manifold variations. The proposed method has a multi-element character discretizing the probability space into simplex elements using a Delaunay triangulation. For every simplex, the high-dimensional solutions corresponding to its vertices (sample points) are projected onto the Grassmann manifold. The pairwise distances between these points are calculated using appropriately defined metrics and the elements with large total distance are sub-sampled and refined. As a result, regions of the probability space that produce significant changes in the full-field solution are accurately resolved. An added benefit is that an approximation of the solution within each element can be obtained by interpolation on the Grassmann manifold. The method is applied to study the probability of shear band formation in a bulk metallic glass using the shear transformation zone theory.

1. Introduction

Over the last several decades, the use of high-dimensional physics-based computational models (high-fidelity models) to assess the behavior of complex physical systems has become ubiquitous. Using models of increasing fidelity for the description of the physical system helps ensure that the requisite information to understand the physics of the system is available but may come at great computational cost. Given uncertainties in the model input or the parameters of the model itself, the problem is set in a probabilistic framework in order to quantify the uncertainty in the behavior/response of the physical system. This process, referred to as uncertainty quantification (UQ) becomes tremendously expensive with the use of high-fidelity models as it requires many repeated model simulations.

Given these computational constraints, it is essential to carefully select the points at which the solution is evaluated. Over the past 20+ years, numerous approaches have been proposed to efficiently sample a probability space in order to reduce the required number of simulations. These methods differ in their approach ranging from those that are statistical in nature (i.e. employing Monte Carlo simulations) to those using so-called surrogate models or reduced-order models (ROMs). Statistical methods generally refer to those methods that sample randomly according to some variance reduction strategy that usually serves to improve the space-filling properties of the samples (e.g. Latin hypercube sampling) [1]. Surrogate modeling approaches aim to develop a simpler mathematical function that is inexpensive to evaluate and accurately

* Corresponding author.
E-mail address: michael.shields@jhu.edu (M.D. Shields).

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Nomenclature

$\bar{\sigma}$	Magnitude of deviatoric stress
$\boldsymbol{\Gamma}$	Matrix representation of a point $\mathcal{H}$ on $\mathcal{T}_{\mathcal{X}}$
$\boldsymbol{\omega}$	spin
$\boldsymbol{\Psi}, \boldsymbol{\Phi}, \mathbf{X}, \mathbf{Y}$	Orthonormal basis on $\mathcal{V}(p,n)$ representing a point on $\mathcal{G}(p,n)$
$\boldsymbol{\Sigma}$	Diagonal matrices of singular values of the solution matrix $\mathbf{F}$
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\boldsymbol{\sigma}_0$	Deviatoric stress
$\boldsymbol{\Theta}$	Diagonal matrix of principal angles θ
$\boldsymbol{\xi}$	Vector of independent random variables uniformly distributed on $[0,1]$
χ	Effective disorder temperature
χ_∞	Saturation value of effective temperature
Δ	Typical activation barrier
$\delta(\boldsymbol{\Psi}_i, \boldsymbol{\Psi}_j)$	Distance between points $\boldsymbol{\Psi}_i$ and $\boldsymbol{\Psi}_j$ on manifolds with different dimensions
$\dot{\mathcal{X}}_0$	Initial derivative for a geodesic path on $\mathcal{G}(p,n)$
ϵ_0	Typical local strain at STZ transition
$\iota_n()$	Inclusion mapping from $\mathbb{R}^n \to \mathbb{R}^{n+1}$
$\mathbb{P}$	Probability measure
$\mathbf{S}$	Diagonal matrices of singular values corresponding to a SVD
$\gamma(z)$	Geodesic path on $\mathcal{G}(p,n)$ indexed on $z \in [0,1]$
$\mathcal{F}$	σ-algebra of events
$\mathcal{G}(,\infty)$	Infinite Grassmann manifold
$\mathcal{G}(\infty,\infty)$	Doubly infinite Grassmann manifold
$\mathcal{G}(p,n)$	Grassmann manifold of p-dimensional subspaces of $\mathbb{R}^n$
$\mathcal{H}$	Subspace of $\mathbb{R}^n$ of dimension p on $\mathcal{T}_{\mathcal{X}}$
$\mathcal{O}(p)$	Orthogonal group of $p \times p$ matrices
$\mathcal{T}_{\mathcal{X}}$	Tangent space at $\mathcal{X}$
$\mathcal{V}(p,n)$	Compact Stiefel manifold of p-dimensional orthonormal bases in $\mathbb{R}^n$
$\mathcal{X}$	Subspace of $\mathbb{R}^n$ of dimension p on $\mathcal{G}(p,n)$
$\mathcal{X}_0$	Initial point for a geodesic path on $\mathcal{G}(p,n)$
$\mathcal{X}_1$	End point for a geodesic path on $\mathcal{G}(p,n)$
μ	Shear modulus
μ_χ	Mean effective temperature
ν	Poisson's ratio
Ω	Sample space
ω_k	Simplex in Ω
$\Omega_+(),\ \Omega_-()$	Schubert varieties
ω_{sub_k}	Sub-simplex of ω_k
ρ	Density
σ	Singular value
σ_χ	Standard deviation of effective temperature
σ_y	Yield stress
τ_0	Molecular vibration timescale
$\mathbf{C}$	Fourth-order elastic stiffness tensor
$\mathbf{D}$	rate-of-deformation tensor
$\mathbf{D}^{el}$	elastic rate-of-deformation tensor
$\mathbf{D}^{pl}$	plastic rate-of-deformation tensor
$\mathbf{F}$	Solution matrix of the full-model of dimension $n_f \times m_f$
$\mathbf{I}_p$	Identity matrix of size p
$\mathbf{Q}$	Orthogonal matrix
$\mathbf{s}$	Vector of random variables arbitrarily distributed on Ω
$\mathbf{U}$	Matrix of left singular orthonormal basis vectors corresponding to a SVD
$\mathbf{V}$	Matrix of right singular orthonormal basis vectors corresponding to a SVD
$\mathbf{v}$	velocity
$\mathbf{v}_{ik}$	Vertex i of simplex ω_k
θ	Principal angle
θ_{ref}	Threshold average principal angle
$\tilde{\boldsymbol{\Phi}}$	Right singular vectors of the interpolated solution matrix $\tilde{\mathbf{F}}$
$\tilde{\boldsymbol{\Psi}}$	Left singular vectors of the interpolated solution matrix $\tilde{\mathbf{F}}$
$\tilde{\boldsymbol{\Sigma}}$	Matrix of singular values of $\tilde{\Gamma}$
$\tilde{\boldsymbol{\Sigma}}$	Matrix of singular values of the interpolated solution matrix $\tilde{\mathbf{F}}$
$\tilde{\Gamma}$	Interpolated point on the tangent space
$\tilde{\Omega}$	Typical activation volume
$\tilde{\mathbf{F}}$	Approximation of the solution matrix $\mathbf{F}$
$\tilde{\mathbf{U}}$	Left singular vectors of $\tilde{\Gamma}$
$\tilde{\mathbf{V}}$	Right singular vectors of $\tilde{\Gamma}$
$\tilde{\theta}$	Average principal angle
$\tilde{d}$	Average total distance across all elements
ε	Machine epsilon
C^{n_d}	Unit hypercube of dimension n_d
c_0	Specific heat-like quantity
c_χ	Coefficient of variation of effective temperature
c_s	Shear wave speed
D_χ	Rate dependent diffusivity
D_k	Total Grassmann distance for element ω_k
$d_{\mathcal{G}(,)}(\boldsymbol{\Psi}_0, \boldsymbol{\Psi}_1)$	Distance on $\mathcal{G}(n,p)$ between points $\boldsymbol{\Psi}_0$ and $\boldsymbol{\Psi}_1$
D_{th}	Threshold total Grassmann distance
E	Elastic modulus
e_z	STZ formation energy
$f_{\mathbf{s}}$	Probability density of parameters $\mathbf{s}$
K	Bulk modulus
k_B	Boltzmann constant
l	Refinement level
l_χ	Length scale of effective temperature variations
l_d	Diffusion length scale
n	Number of degrees of freedom
n_c	Number of candidate elements for refinement
n_d	Number of random variables
n_e	Number of elements
$n_f \times m_f = n$	Dimension of the solution matrix
n_s	Number of samples
n_{ref}	Number of elements selected for refinement
$O()$	Asymptotic notation
r	Rank of a matrix
S	Parameter space
S_c	Configurational entropy
T	Temperature
t	time
U_B	velocity of boundaries
U_c	Configurational energy
U_c	Potential energy
V_{ω_k}	Volume of element ω_k
tol	Tolerance threshold for SVD